Knots in soft condensed matter

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The full potential of fundamental research is sometimes only realised a long time after the work was initiated, and may take a form that could not have been predicted at the outset. This has certainly been the case for research on the scientific properties of knots. The first systematic tabulations of knotted topologies were carried out by P. G. Tait [1] in the late nineteenth century, motivated by the long-since abandoned vortex theory of atoms [2] due to William Thomson (later created Lord Kelvin). Fortunately, the demise of Thomson's theory did not deter mathematicians from developing a sophisticated understanding of the topological properties of knots in their own right (for an accessible introduction, see the book by Adams [3]). The resulting theoretical framework is now finding applications in a wide range of fields in the physical sciences that could not even have been imagined when Tait was carrying out his seminal investigations.

Because of the diversity of sub-disciplines in which knots are playing an increasingly important role, developments in one area are not always communicated to others where they may be relevant. The aim of this Special Issue of *Journal of Physics: Condensed Matter* is to promote cross-fertilisation of ideas between research communities by gathering together the latest contributions to some of the major contemporary knot-related topics in condensed matter. In a similar spirit, a CECAM workshop entitled *Knots in Soft Condensed Matter* was held from 10 to 13 September 2014 at the University of Vienna to provide a forum for direct discussions. Topics represented at the meeting were diverse: linear and ring polymers, proteins, DNA, liquid crystals, soap films, organic synthesis, magnetohydrodynamics, and toplogical glasses, as well as matters of more general analysis such as entangled networks and methods for loop closure. This issue includes accounts some of the work that was presented at the Vienna meeting but is not restricted to it.

One of the broad themes that emerges from the collection of articles presented here and from the CECAM meeting is a drive to understand how dynamic processes affect, and are affected by knots. Indeed, this Special Issue could almost have been entitled "Knots in action". While questions of structure can often be considered in general or abstract terms, it is usually harder to separate questions of dynamics from the physical nature of the system in which they occur. Hence, the consequences of knotted topology are particularly rich when it comes to dynamic properties, and the manifestation of knots in real physical systems can give rise to interesting new phenomena, as illustrated by the articles in this Special Issue.

Knotted molecules of various kinds feature strongly in the collection of articles, and the Issue opens with a wide-ranging review by Lim and Jackson [4] on the structure, formation and properties of molecular knots, covering DNA, RNA, proteins and synthetic molecular knots.

Three of the research articles focus on knots in DNA. Suma et al. [5] use Langevin dynamics simulations to look at spontaneous knot formation in DNA chains confined inside nanochannels of width comparable to the DNA persistence length. The study focuses, in particular, on the very different time scales associated with the lifetimes of knotted and unknotted states in DNA chains of different lengths, and relates them to the occurrence of backfolding events at the chain ends. Liu and Chan [6] propose a model for how type-2 topoisomerases might harness local geometrical features or supercoiled DNA

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filaments to carry out the selective strand passages required to control the linking number distribution. Building on their previous work, the authors suggest that the local geometrical clues exploited by the topoisomerases arise from the geometrical variations of the so-called hooked DNA juxtapositions. Uehara and Deguchi [7] use stochastic simulations to sample the equilibrium population of DNA rings and establish the incidence of knots upon varying both the contour length of the rings and also their thickness (which captures the effective electrostatic screening operated by counterions). The data are used to establish the characteristic length scales that govern the decay of the unknotted population upon increasing chain length at fixed thickness.

New work on knotted proteins is presented in five papers, covering both experiments and simulations. Chwastyk and Cieplak [8] present a molecular dynamics study of the folding of knotted proteins using structure-based potentials. Thanks to the computationally accessible model, they are able to show how the knot formation probability is enhanced by the simultaneous folding and synthesis of the protein from the ribosome. Wang et al. [9] present an experimental study of the variants of the HP0242 protein from *Helicobacter pylori*. By employing a variety of spectroscopic tools, the authors have systematically characterised the folding–unfolding transition of HP0242 variants. The analysis of the equilibrium and kinetic properties reveals a complex refolding pathway, that has long-lived intermediates essential for proper folding, but is fast compared to many other known knotted proteins. Haglund [10] discusses the importance of entangelment stabilised by covalent disulfide bonds in the biological function of single proteins. The fascinating message is that disulfide bonds act as on/off switches for pierced lasso bundles, not only affecting the state of the protein but also acting as sensors for the reductive power of the cell. Burban et al. [11] present an experimental NMR study of refolding in the minimal tied trefoil protein. The work identifies the role of side-chain contacts, and in particular the influence of proline 62. Relaxation of this residue from the native-state *trans* conformation to a *cis* conformation when denatured, induces strong hysteresis in the unfolding–folding cycle. In a computational study, Dabrowski-Tumanski et al. [12] pick apart the interactions in the smallest knotted protein (2efv in the Protein Data Bank) to determine how they affect knotting and folding. The native contact interactions are sufficient for the knotted structure to fold, but an additional subset of "native-like" contacts in the loop region greatly enhances the kinetics, and certain non-native contacts accelerate the rate still further.

Moving away from properties of individual molecules, two articles provide contrasting illustrations of more collective phenomena that result from knotted topology. Trefz and Virnau [13] use extensive molecular dynamics simulations to sample the conformational space of ring polymers of different topology in melts. They examine the scaling properties both of the size of the rings and of their knotted portion. Ravnik et al. [14] consider the defects created by colloidal inclusions in a nematic liquid crystal. In particular, they examine the modifications of the defect lines introduced when the colloidal particles change their shape and genus, and discuss the observed variety of ensuing complex topologies.

On a more abstract note that is relevant to knots in any context, Hyde et al. [15] devise methods for assessing knot complexity by showing how the topology of a knot emerges from the topology of segments of the structure as the length of the segment is continuously increased. The resulting fingerprints provide a visualisation of fine structure and can be mapped onto a planar graph for further analysis. Although the article concentrates on tight knots, the methods can be applied to any closed curve.

We hope that this collection of articles will provide a valuable point of reference as research on knots continues apace. We are grateful to the editorial board and staff of *Journal of Physics: Condensed Matter* for their support in preparing this Special Issue, and we thank all the authors for their contributions.

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